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# A Generic Combined Matrix- and Lattice-Based Kinetic Monte Carlo Modeling Tool to Tune Surface-Initiated Polymerization †

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The development of biofunctionalized polymer interfaces through the deposition of bio-derived polymeric layers to flat surfaces has attracted much attention, due to the wide range of potentially relevant applications. Examples are the production of coatings for protection against corrosion, novel adhesive materials, protein resistant bio-surfaces, chemical lubricants, and polymer-carriers for the controlled release of active compounds, which are derived from the highly efficient adaptation of physicochemical properties of these surfaces. Mostly, these polymeric layers are produced by a grafting-from-synthesis strategy, wherein polymer chains are produced in situ from suitable polymerization initiator molecules previously attached to the surface, resulting in a surface with a high grafting density of initiating sites. This synthesis strategy can be accomplished by implementing different surface-initiated polymerization mechanisms, including living cationic and anionic polymerization, as well as surface-initiated reversible deactivation radical polymerization that enables the production of "green" biopolymeric materials from environmentally friendly chemical sources. One of the most important challenges to face during the preparation of the polymer layer is to perform a thorough characterization based on the molar mass and dispersity on the individual chain level, as well as the variation of its thickness as a function of the polymerization time and the grafting density, which define the mushroom/brush character of the biofunctionalized polymer interface. Such characterization, however, is a cumbersome task to perform solely based on experimental studies. These limitations can be circumvented from the implementation of advanced computational modeling tools that enable the extensive in silico characterization of the desired polymerization products. In this context, a generic matrix-based kinetic Monte platform has been developed by our group [1,2], capable of evaluating the three-dimensional growth pattern of the individual polymer chains within the (biofunctionalized) polymer interface. It allows for a detailed study of the conformation of the polymer chains and other relevant molecular properties, enabling the optimization of the synthesis conditions and control strategies for the production of well-defined polymer interfaces.

**Keywords:** stochastic modeling; surfaces; conformations; kinetics; apparent livingness

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